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厦门大学

博　士　学　位　论　文

低维晶格模型的热传导问题研究

Thermal Conduction in Low-dimensional Lattice Models

钟　毅

指导教师姓名：赵　鸿　教授
专　业 名 称：理　论　物 理

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摘　要

本论文研究非对称相互作用势对低维材料热传导性质的影响。近年来，低维材料的热输运性质已经成了人们研究的热点，其中一个主要的目的是检验傅立叶定律在低维材料中是否适用。众所周知，热传导中的傅立叶定律是一个重要的基本规律。它指出材料的热流正比于温度梯度： $J=-\kappa\nabla T$ ，其中 κ 是一个有限的常数，称之为热导率。如果热传导行为遵循傅立叶定律，那我们称之为正常热传导；否则称为反常热传导。目前，流体力学方法和模耦合理论等理论分析方法都给出基本一致的预测，即低维情况下动量守恒系统的热导率随系统尺寸发散：一维以幂指数方式发散；二维以对数方式发散。此外，在 2000 年，Prosen 和 Campbell 也在理论上证明了，对于动量守恒但是内压力不为零的一维系统，它的热导率在热力学极限下是发散的。然而，我们知道内压力不为零的系统代表非对称势，它会使材料产生热胀冷缩效应，而真实材料通常都有热胀冷缩效应并且热传导行为也遵从傅立叶定律，这激发我们去研究非对称相互作用势在低维材料的热传导中所扮演的角色。

本文首先用非平衡态的方法研究了非对称相互作用势下一维材料的热传导规律。我们构造了一个含可调参数 r (用来调节非对称度)的非对称相互作用势。通过调节非对称参数，我们发现，在适当的非对称度和一定的温度下，系统表现为正常热传导行为，即它满足傅立叶定律。通过计算系统在非平衡态下的质量密度分布，我们发现非对称势系统有质量密度梯度，而对称势系统没有。我们认为，质量密度梯度为热流提供了额外的散射机制，结合非线性作用导致的声子散射机制，共同导致了正常热传导行为。

在此基础上，本文进一步用平衡态下 Green-Kubo 公式计算了一维非对称相互作用势晶格的热导率。首先我们让系统演化到平衡态，然后计算了热流自关联函数 $C(t)/N=\langle J(t)J(0)\rangle/N$ ，其中 $J(t)$ 是 t 时刻总热流， N 是系统尺寸。我们的计算结果表明，在不同系统尺寸下 $C(t)/N$ 的曲线都是重合的，并且衰减速度要比幂律 $C(t)/N\sim t^{-1}$ 更快，这说明系统有正常热传导行为。因此，平衡态方法与

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非平衡态方法都证明非对称相互作用势可以导致正常热传导。更进一步，为了区分是非对称度性还是非谐性导致系统正常热传导行为，我们考察了非对称简谐振子系统，结果表明，是非对称度导致了正常热传导行为。同时，本文初步研究了非对称势系统的能量密度涨落时空关联函数。模拟结果显示，非对称势系统的时空关联函数其瑞利峰是高斯波包，与对称系统的瑞利峰定性不同。这也预示了非对称势系统具有正常热传导行为。

最后，本文初步研究了二维非对称势下晶格系统的热传导规律。计算结果显示这些系统也有正常热传导行为。我们在一维和二维非对称势系统中的发现，对于真实材料而言有重要的意义：它意味着真实的低维材料在热力学极限下同样遵从傅立叶热传导定律，和三维材料一样具有尺寸无关的热导率。

关键词： 非对称相互作用势；热传导；Green-Kubo 公式；非平衡统计

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Abstract

We investigate the effects of asymmetric interparticle interactions on thermal conduction of low-dimensional momentum conserving lattices. In recent years, the property of thermal transport in low-dimensional material has attracted intensive studies, one of the issues is to verify the validity of the Fourier's law for thermal conduction. As we all known, the Fourier' law of thermal conduction is a fundamental theorem in physics. It states that the heat flux J in material is proportional to the temperature gradient ∇T, i.e., $J=-\kappa\nabla T$, where κ is a finite constant termed as "thermal conductivity". The systerm has "normal heat conduction" if thermal conduction behavior obeys the Fourier's law. Otherwise, it has so-called "anomalous heat conduction". Several analytical methods have been proposed so far, such as the hydrodynamic approach and the mode-coupling theory. They all predict that thermal conductivity diverges with the system size in a power (logarithmic) law in 1D(2D) momentum conserving systems. In addition, Prosen and Campbell also proved theoretically that thermal conductivity diverges in the thermodynamic limit for 1D momentum conserving lattices with nonvanishing internal pressure. However, it is well-known that a lattice with nonvanishing internal pressure imply the interparticle interaction is asymmetric, which can induce thermal expansion. And real materials usually show the thermal expansion effect and obey the Fourier's law. Thus, we need to investigate the effects of asymmetric interparticle interactions on thermal conduction of low-dimensional momentum conserving lattices.

In this thesis, we firstly study thermal conduction in 1D momentum conserving lattices with asymmetric interparticle interactions by nonequilibrium molecular dynamics simulations. We construct an

asymmetric potential with a parameter r to control the degree of the asymmetry. We found that system with appropriate asymmetry exhibits normal thermal conduction at a certain temperature. We also found that the asymmetric interaction can give rise to a mass gradient across the system while the symmetric one can not. Therefore, we conjecture that the mass gradient can induce additional scattering of the heat flux and, together with other scattering mechanism, result in the occurrence of normal thermal conduction.

Based on the results above, we calculate thermal conductivity by using the Green-Kubo formula so as to verify our finding that asymmetric interactions in 1D momentum conserving lattices can induce normal heat conduction. At first, evolve the system for a sufficient long time so as to relax the system to its equilibrium state. We then calculate the current correlation function $C(t)/N = \langle J(t)J(0)\rangle / N$, where $J(t)$ is the total heat flux at time t, N is the system size. Our equilibrium simulations show that the curves of $C(t)/N$ for different sizes are consistent with each other. And they decay faster than the power-law decay, i.e. $C(t)/N \sim t^{-1}$, implying a convergent thermal conductivity. Thus, the conclusion that the asymmetric interaction can result in normal thermal conduction is verified by both equilibrium and nonequilibrium simulations. Furthermore, in order to clarify whether the normal thermal conduction is resulted by the anharmonicity or the asymmetry feature, we study the asymmetric harmonic systems. The results confirm that it is the asymmetry of interaction potentials that result in the normal heat conduction. At the same time, we preliminarily study the spatiotemporal correlation of the energy density fluctuations in the asymmetric interaction lattices. Our simulations show that the Rayleigh peak of the spatiotemporal correlation function in the lattice of asymmetric interaction is Gaussian wave packet,

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while the lattice of symmetric interaction shows non-Gaussian wave packet. It also indicates the lattice of asymmetric interaction has normal thermal conduction.

Finally, we preliminarily study thermal conduction in 2D momentum conserving lattices with asymmetric interparticle interactions. The numerical results show that these lattices also have normal thermal conduction. The findings in 1D and 2D momentum conserving lattices with asymmetric interactions are important for understanding the thermal property of real materials. It implies that low-dimensional materials may also have the finite thermal conductivity in the thermodynamic limit as the bulk materials, and the Fourier's law of heat conduction is generally valid for low-dimensional materials.

Keywords: asymmetric interparticle interaction; heat conduction; Green-Kubo formula; nonequilibrium statistical physics

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